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Crossover behavior in quantum nonlinear resonance in a hydrogen atom

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Abstract

We consider the slow dynamics of a Rydberg electron in a hydrogen atom driven by a resonant microwave field. Two crossovers in this system are discussed as the amplitude ϵ of the external field increases. The first one creates isolated quantum nonlinear resonance (QNR) [see G.P. Berman and G.M. Zaslavsky, Phys. Lett. A 61 (1977) 295]. The second crossover occurs when the QNRs overlap and a transition to chaos takes place. We analyze numerically the dependence $\delta n(\epsilon)$ in the regions of these two crossovers, where δn is the characteristic number of unperturbed levels (or quasienergies) trapped in the potential well of the QNR, and discuss the possibility of observing these crossover effects experimentally.

1. Introduction

When a quantum system with a non-equidistant spectrum is driven by a resonant external field, quantum nonlinear resonance (QNR) may occur, as introduced in [1]. A QNR is characterized by two main parameters: the number of quasienergy levels δn which are trapped into the potential well of the resonance (the value of δn also characterizes the number of levels of the unperturbed Hamiltonian involved in the dynamics), and the characteristic frequency of slow oscillations Ω_{ph}. QNR in such a system is the quantum analog of nonlinear resonance (NR) which would occur in the corresponding classical system [2,3]. NR plays an important role in classical dynamical Hamiltonian systems, and describes, roughly speaking, a stable "quasiparticle" (undestroyed KAM-torus [2]) in the classical phase space. QNR is a very general phenomenon in quantum dynamical systems with non-equidistant spectra [1,4–8]. Namely, an individual (isolated) QNR describes a stable quantum system [1], and overlapping of the QNRs causes a transition to quantum chaos [4–8]. Experimental observation of QNR would be of significant interest. Some problems connected with experimental observation of QNR were discussed in [9]. Direct observation of QNR requires to study the two main parameters of QNR mentioned above: δn and Ω_{ph}. One of the potentially observable features of QNR is connected with the crossover in the dependence of $\Omega_{\text{ph}}(\epsilon)$, where ϵ is a dimensionless amplitude of an external resonant field. Namely, when ϵ is small enough, and a two-level approximation can be used, then $\Omega_{\text{ph}} \sim \Omega_{\text{R}} \sim \epsilon$, where Ω_{R} is the resonant Rabi frequency (see, for ex-

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ample, [10]). When the amplitude of the resonant microwave field increases, and an isolated QNR occurs, the dependence $\Omega_{\rm ph}(\epsilon)$ changes, to become $\Omega_{\rm ph}(\epsilon) \sim \sqrt{\epsilon}$. This crossover effect in the dependence $\Omega_{\rm ph}(\epsilon)$ could be experimentally measurable. However, an experimental measurement of the quasienergies is rather complicated, and requires a separation of the characteristic quasienergy of the QNR $\Omega_{\rm ph}$ from all others. Instead, we consider numerically in this paper a characteristic of the QNR which could be experimentally observable in a hydrogen atom interacting with a microwave resonant field, and is connected with the dependence $\delta n(\epsilon)$ of the number of quasienergy levels on the amplitude of the external field. As we shall show, the quantity $\delta n(\epsilon)$ in being "integral" is a robust characteristic feature of the QNR, and may be observable in experiments with Rydberg hydrogen atoms in a resonant microwave field.

2. The main equations and the numerical results

Let a microwave electric field $\boldsymbol{E}(t) = \boldsymbol{e}_z E_0 \cos \omega t$ be polarized along the z-axis, and $\boldsymbol{r}$ be an electron radius-vector in the hydrogen atom. Then, the interaction of a microwave field with an electron is described by the matrix elements $\langle \mathbf{H}_{\rm int}\rangle(t) = -E_0 \cos \omega t \langle n', l', m | d_z | n, l, m\rangle$, where $d_z = er_z$ is the z-component of the atomic dipole moment, the integers n', n are the principle quantum numbers, l', l are the orbital angular momentums quantum numbers, and m is projection of the orbital angular momentum on the z-axis. We shall consider only those transitions which correspond to $n' \sim n \gg 1$, and to small orbital angular momenta: $l', l \ll n', n$. These conditions mean that the electron trajectories are nearly one-dimensional (see, for example, the review [11], and references therein). Let the complex amplitude of the electron population be $c_{n,l,m}(t)$, satisfying the Schrödinger equation with the interaction Hamiltonian above. Introduce the complex amplitudes $\eta_n(t) = \sum_l c_{n,l,m}(t)$, and consider the transitions only with $n' = n \pm 1, n \pm 2$. Then, taking into account the conditions mentioned above, we derive the following equations for the amplitudes $\eta_n(\tau)$:

$$i\frac{d\eta_n}{d\tau} = -\frac{1}{2n^2}\eta_n + i\epsilon \cos \nu\tau \{\lambda(n-1)^2\eta_{n-1} + \mu(n-2)^2\eta_{n-2} - \lambda n^2 \eta_{n+1} - \mu n^2 \eta_{n+2}\}, \tag{1}$$

where $\lambda = J_1'(1)$, and $\mu = \frac{1}{2}J_2'(2)$, and $J_k'(x)$ is the first derivative of the Bessel function $J_k(x)$. In (1) ϵ, ν, τ are the dimensionless amplitude of the external field, microwave frequency, and time. Eq. (1) describes the quantum dynamics of an electron, provided the amplitude of the external field is small enough, $\epsilon < \epsilon_{\rm cr}^{(2)}$, for an isolated quantum nonlinear resonance (QNR) occurs. An equation which describes the slow quantum dynamics of QNR can be derived from (1) in the following way (see also [1,4]). Expand the unperturbed energy spectrum $E_n = -1/2n^2$ in the vicinity of a resonant level n_0 (see below) up to the first nonlinear term

$$E_n \approx E_{n_0} + \omega_{n_0}(n - n_0) - \tfrac{1}{2}\gamma(n-n_0)^2,$$
$$E_0 \equiv -1/2n_0^2, \quad \omega_{n_0} \equiv 1/n_0^3, \quad \gamma \equiv 3/n_0^4. \tag{2}$$

In the quasiclassical region ($n \gg 1$), and under the condition of small enough ϵ, we may take into consideration only transitions with $n' = n \pm 1$. Then, in the resonant approximation $|\Delta| \ll \omega_{n_0}, \nu$ ($\Delta = \nu - \omega_{n_0}$) we derive from (1) the equations for the slow amplitudes,

$$iA_m \approx -\tfrac{1}{2}\gamma m^2 A_m + \tfrac{1}{2} i\epsilon n_0^2 \lambda (e^{-i\Delta\tau}A_{m-1} - e^{i\Delta\tau}A_{m+1}),$$
$$\eta_n(\tau) = A_m(\tau)\exp\{-i[E_0 + \omega_{n_0} m]\} \quad (m = n - n_0). \tag{3}$$

Eq. (3) can be written in the form of the Schrödinger equation

$$i\frac{\partial\Phi}{\partial\tau} = \tfrac{1}{2}\gamma\frac{\partial^2\Phi}{\partial\theta^2} - \epsilon n_0^2 \lambda \sin(\theta - \Delta\tau)\Phi,$$
$$\Phi(\theta,\tau) = \Phi(\theta + 2\pi, \tau) = \sum_m A_m(\tau) e^{im\theta}. \tag{4}$$

Upon introducing the new variables $\tau' = -\tau$, and $\vartheta = \theta - \Delta\tau - \pi/2$, we derive from (4) the following time-independent Schrödinger equation for the QNR:

$$i\frac{\partial\Phi}{\partial\tau'} = \hat{H}_{\rm QNR}\Phi,$$

$$\hat{H}_{\mathrm{QNR}} = \Delta \hat{I} + \tfrac{1}{2}\gamma \hat{I}^2 - \epsilon n_0^2 \lambda \cos \vartheta \qquad \left(\hat{I} \equiv -i\frac{\partial}{\partial \vartheta} \right). \tag{5}$$

In the classical limit the operator $\hat{I}$ reduces to the classical action I, and the classical Hamiltonian of the nonlinear resonance (NR) has the form

$$H_{\mathrm{NR}} = \Delta I + \tfrac{1}{2}\gamma I^2 - \epsilon n_0^2 \lambda \cos \vartheta. \tag{6}$$

The quasiclassical quantization for the QNR takes the form $\int_0^{2\pi} I(\vartheta, \varepsilon_n) d\vartheta = 2\pi n$, where ε_n is the quasienergy spectrum of the QNR. The quasienergy spectrum of an isolated QNR, and two interacting QNRs are discussed in [6–8,12].

As one can see from (5), (6), the characteristic frequency of the QNR Ω_{ph} is of order $\Omega_{\mathrm{ph}} \approx \sqrt{\epsilon \gamma \lambda n_0^2}$ [1,2]. This means that the characteristic frequency of the slow oscillations Ω_{ph} in the vicinity of the QNR depends on the amplitude of the external microwave field ϵ according to the law $\Omega_{\mathrm{ph}}(\epsilon) \sim \sqrt{\epsilon}$. At the same time, when the amplitude of the external resonant field is sufficiently small ($\epsilon \ll \epsilon_{\mathrm{cr}}^{(1)}$), we may use in (1), (2) the two-level approximation. In this case the slow dynamics in the quasiclassical region is described by the Rabi frequency [10]: $\Omega_{\mathrm{R}} = \sqrt{\Delta^2 + \epsilon^2 \lambda^2 n_0^4}$. When the resonance is rather narrow: $|\Delta| \ll \epsilon \lambda n_0^2$, the Rabi frequency is proportional to the first degree of the amplitude of the external field ϵ: $\Omega_{\mathrm{R}} \sim \epsilon \lambda n_0^2$. So, a crossover exists in the dependence of the characteristic frequency of the low oscillations Ω_{ph} on ϵ at some value $\epsilon_{\mathrm{cr}}^{(1)}$, such that at $\epsilon < \epsilon_{\mathrm{cr}}^{(1)}$: $\Omega_{\mathrm{ph}} \sim \epsilon$; and at $\epsilon > \epsilon_{\mathrm{cr}}^{(1)}$: $\Omega_{\mathrm{ph}} \sim \sqrt{\epsilon}$. This crossover in the dependence $\Omega_{\mathrm{ph}}(\epsilon)$ should be experimentally observable.

It is simpler, however, to observe this crossover by investigating the dependence $\delta n(\epsilon)$, where δn is the characteristic number of levels involved into the quantum dynamics of the QNR. As follows from the above considerations, for $\epsilon < \epsilon_{\mathrm{cr}}^{(1)}$ the characteristic number of the trapped into the QNR levels is of order: $\delta n \approx 2$. On the other hand, when $\epsilon > \epsilon_{\mathrm{cr}}^{(1)}$ the dependence $\delta n(\epsilon)$ has the form: $\delta n(\epsilon) \approx (2/\pi)\Delta I \sim \sqrt{\epsilon}$, where $\Delta I = 4\sqrt{\epsilon n^2 \lambda / \gamma}$ is the width of the classical NR in action. So, the first crossover in the dependence $\delta n(\epsilon)$ takes place at the value $\epsilon = \epsilon_{\mathrm{cr}}^{(1)}$. The second crossover in the dependence $\delta n(\epsilon)$ should be expected at some value $\epsilon_{\mathrm{cr}}^{(2)} > \epsilon_{\mathrm{cr}}^{(1)}$ when different QNRs are overlapping, and the transition to quantum chaos takes place. When $\epsilon > \epsilon_{\mathrm{cr}}^{(2)}$, the number of trapped levels should increase significantly with an increase of ϵ.

We should note here that the dependence $\delta n(\epsilon) \sim \sqrt{\epsilon}$, which corresponds to the isolated QNR, is actually quasiclassical, and requires $\delta n \gg 1$. At the same time, as one can easily see, the Rydberg electron in a hydrogen atom, with a principal quantum number $n_0 \approx 70$, and influenced by a resonant microwave field, is not the best quasiclassical system to observe an isolated QNR. Consider the distance between the main QNR centered at the level $n_0^{(1)}$ defined by the equation $1/[n_0^{(1)}]^3 \approx \nu$, and a second QNR, centered at the level $n_0^{(2)}$, and defined by the equation $2/[n_0^{(2)}]^3 \approx \nu$. Then, the distance between these two resonances is $\Delta n \equiv n_0^{(2)} - n_0^{(1)} \approx (\sqrt{2} - 1) n_0^{(1)}$. From this there follows an estimate for the characteristic number of levels trapped into the main QNR under the condition that this resonance is isolated: $\delta n \approx \frac{1}{2}(\sqrt{2} - 1) n_0^{(1)}$. If we choose $n_0^{(1)} = 70$, then $\delta n \approx 9$ (see Fig. 1). This means that the quasiclassical dependence $\delta n \sim \sqrt{\epsilon}$ will not be very well represented in this system. Nevertheless, the results of the numerical calculations show (see below), that this dependence could still be extracted.

The results of the numerical calculations of the dependence of the difference in atomic occupation numbers on the external field amplitude $\delta n(\epsilon) = n_+(\epsilon) - n_-(\epsilon)$ are shown in Figs. 1a,b. In this numerical experiment we used the system of Eqs. (1). The level n_+ is the upper excited level, and the level n_- is the lower excited level. All levels with $|\eta_n|^2 > 0.01$ were included in the dependence $\delta n(\epsilon)$ represented in Figs. 1a,b. The levels with $|\eta_n|^2 < 0.01$ were not included (although they were also calculated). As one can see from Figs. 1a,b, there exists a characteristic dependence $\delta n(\epsilon) \sim \sqrt{\epsilon}$ that corresponds to the isolated QNR for sufficiently low external field amplitude. Also, the second crossover at $\epsilon = \epsilon_{\mathrm{cr}}^{(2)}$ is seen, when different QNRs overlap, and a transition to quantum chaos should occur. Fig. 1a corresponds to the case $\omega_{n_0} \approx \nu$, and Fig. 1b corresponds to the case $\omega_{n_0} \approx 3\nu$. In both cases $n_0 = 70$. The dependence $\delta n(\epsilon)$ presented in Figs. 1a,b is the dependence, we

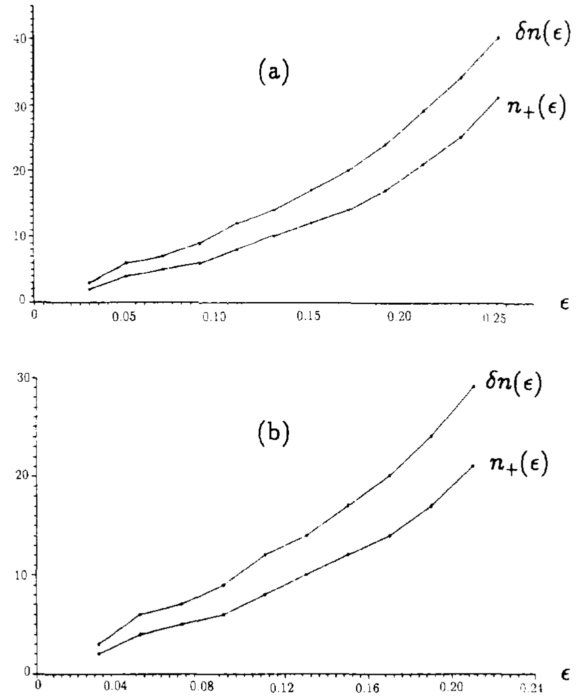

Fig. 1. Dependences $\delta n(\epsilon)$ and $n_+(\epsilon)$ which characterize (breaks in slope) the quantum nonlinear resonance with $\delta n(\epsilon) \sim \sqrt{\epsilon}$, and two crossovers which take place near $\epsilon_{cr}^{(1)} \sim 0.05$ and $\epsilon_{cr}^{(2)} \sim 0.08$; in (a) and (b), respectively, for $n_0 = 70$; (a): $\omega_{n_0} \approx \nu$; (b): $\omega_{n_0} \approx 3\nu$. We suggest in the text that these breaks in the slope of $\delta n(\epsilon)$ and $n_+(\epsilon)$ should be measurable indications of quantum nonlinear resonance and overlap and, thus, creation of QNR at $\epsilon_{cr}^{(1)}$ and overlap, leading to transition to quantum chaos at $\epsilon_{cr}^{(2)}$, in the dynamics of Rydberg atoms driven by a resonant external field of amplitude ϵ.

suggest, that should be investigated experimentally in order to observe QNR using the Rydberg states of a hydrogen atom interacting with a resonant microwave field.

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